Multigrid solution methods for nonlinear time-dependent systems

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Objectives

To solve complex non-linear parabolic systems by applying:

- 2^{nd} order central Finite Difference Method (FDM)
- 2^{nd} order Backward Differentiation Formula (BDF2)
- Nonlinear multigrid method with Full Approximation Scheme (FAS)
- Adaptive Mesh Refinement (AMR)
- Adaptive time-stepping
- Parallel technique

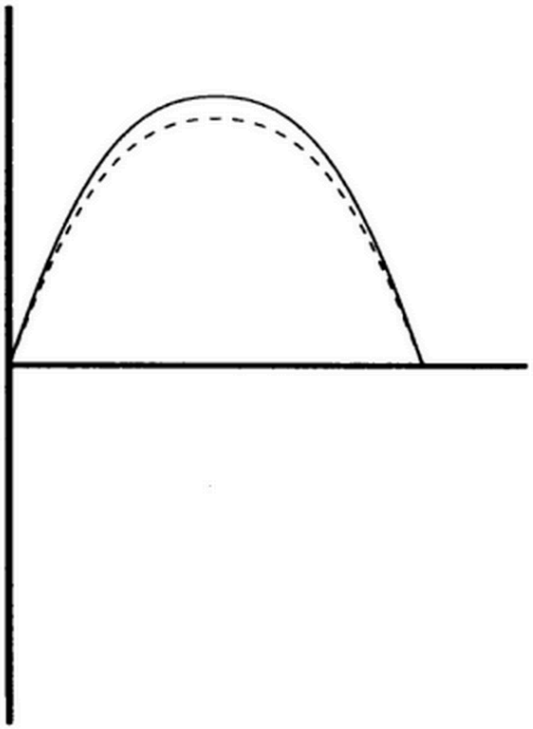
Outline

- Multigrid methods
  - Linear multigrid
  - Nonlinear multigrid
- Thin film models from Gaskell et al.
- Adaptive multigrid solver
- Cahn-Hilliard-Hele-Shaw system of equations from Wise
- Tumour modelling
- Tumour model from Wise et al.
- 2^{nd} order convergence rate
- 3-D results

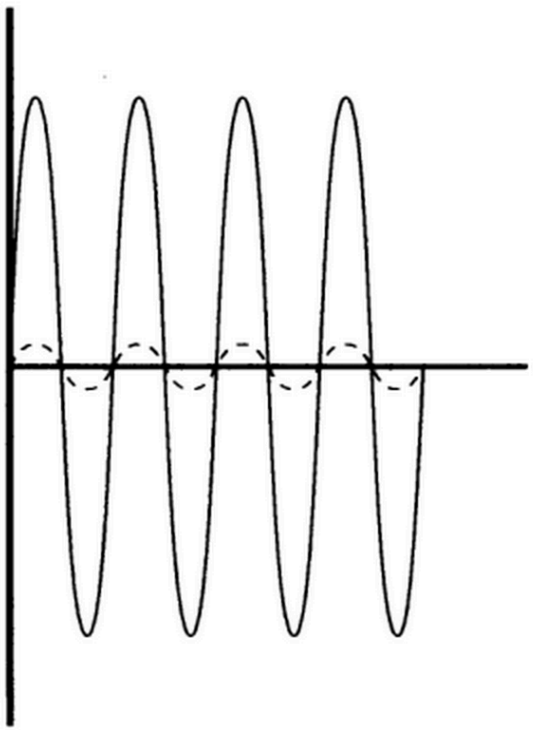
Jacobi/Gauss-Seidel iterative methods

- Well-known methods
- Require diagonally-dominant matrices
- Typically have complexity of $\mathcal{O}(n^2)$ for general sparse matrices
- ...
- Smoothing property

Low frequency of error

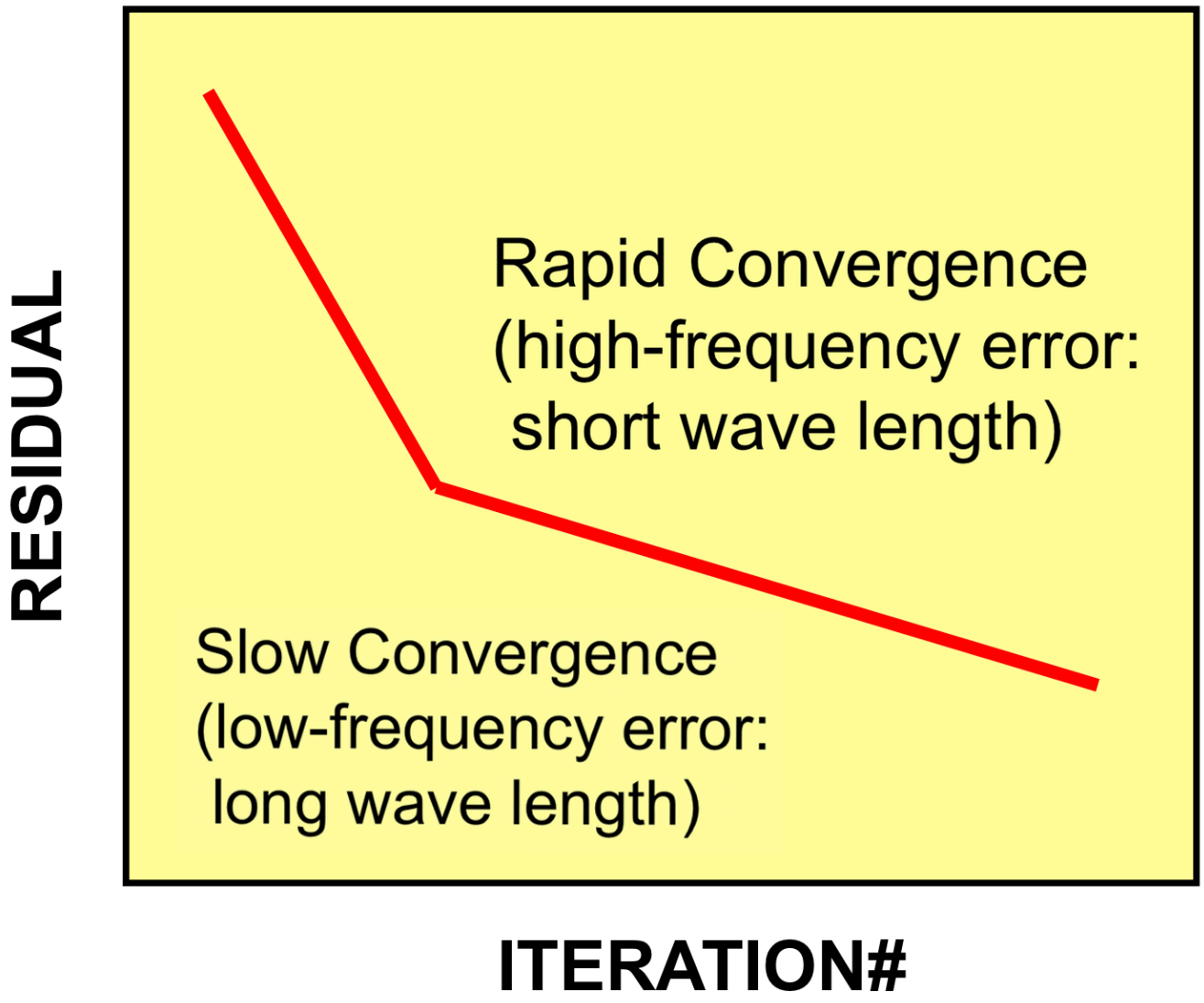


High frequency of error



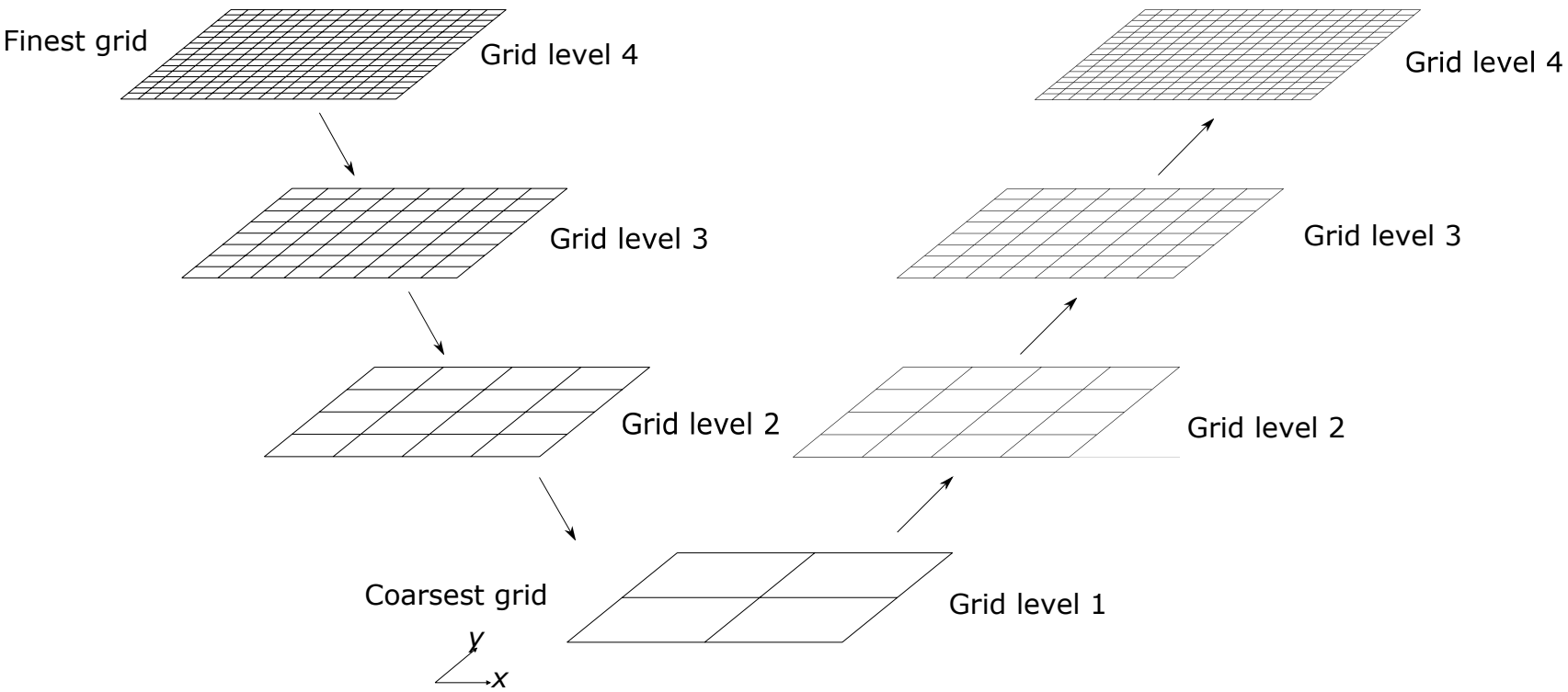
S.H. Lui *Numerical Analysis of Partial Differential Equations*, 2011

Convergence of a typical Jacobi iterative method



source: nkl.cc.u-tokyo.ac.jp

Multigrid v-cycle



Linear multigrid

A linear problem:

$$Au = b, \tag{1}$$

exact error can be obtained as

$$E = u - v, \tag{2}$$

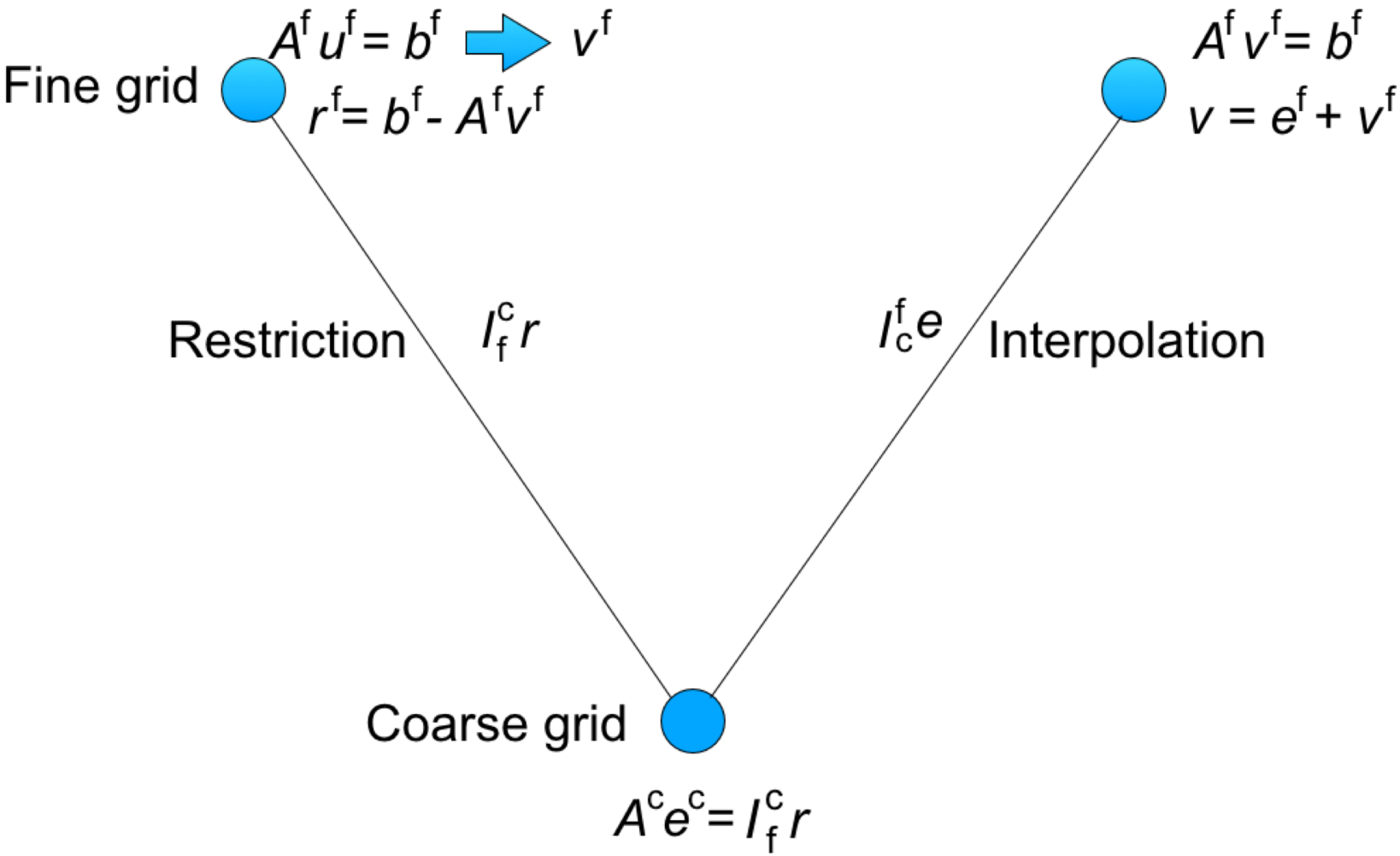
residual can be calculated as:

$$r = b - Av. \tag{3}$$

Error equation:

$$\begin{aligned} AE &= A(u - v) \\ &= Au - Av \\ &= b - Av \\ &= r. \end{aligned} \tag{4}$$

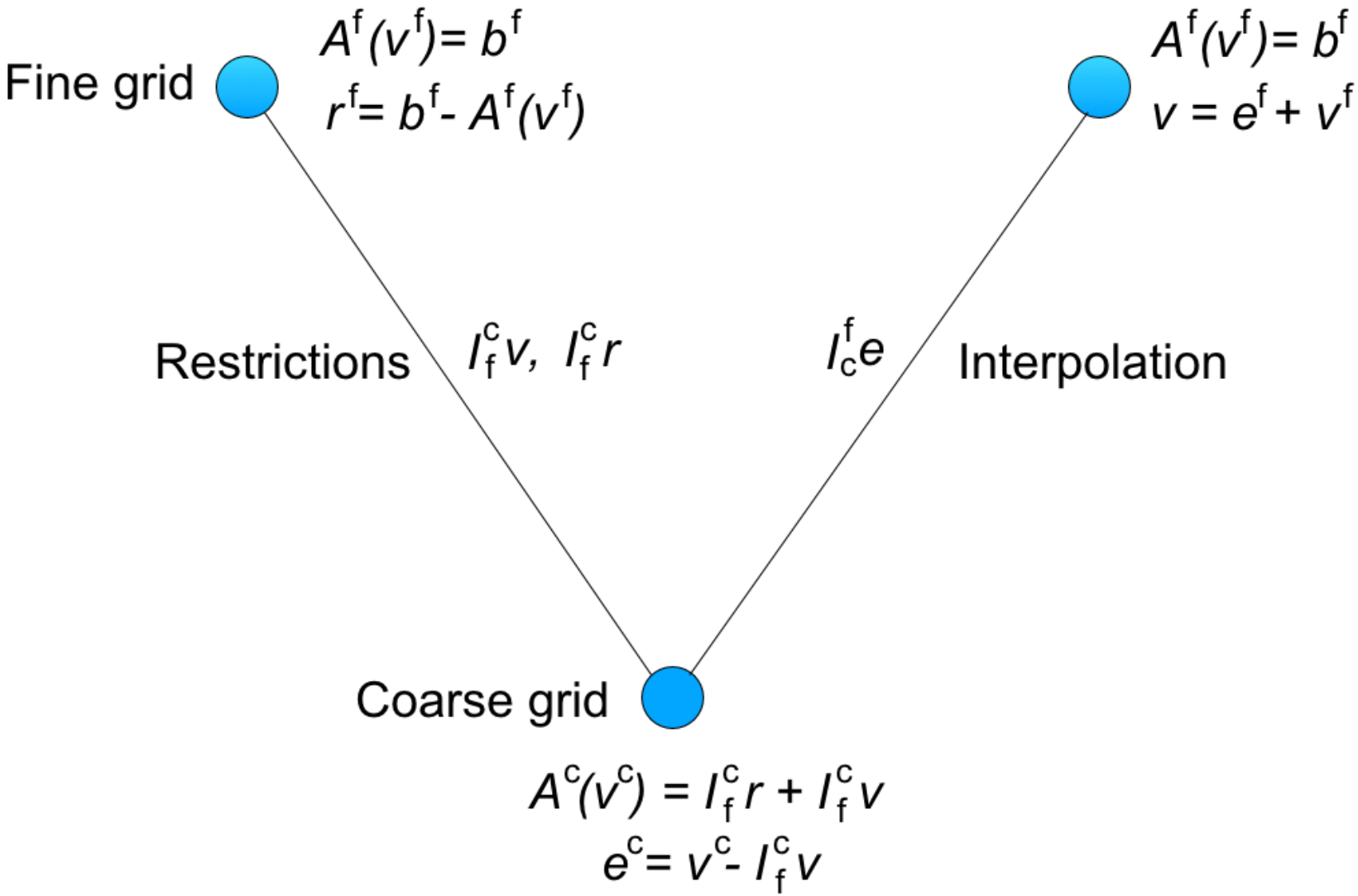
Linear multigrid



Nonlinear multigrid

- The Error Equation (4) does not exist in a nonlinear case
- Full Approximate Scheme (FAS)
- For problem on coarser grids, a modified RHS is included

Nonlinear multigrid

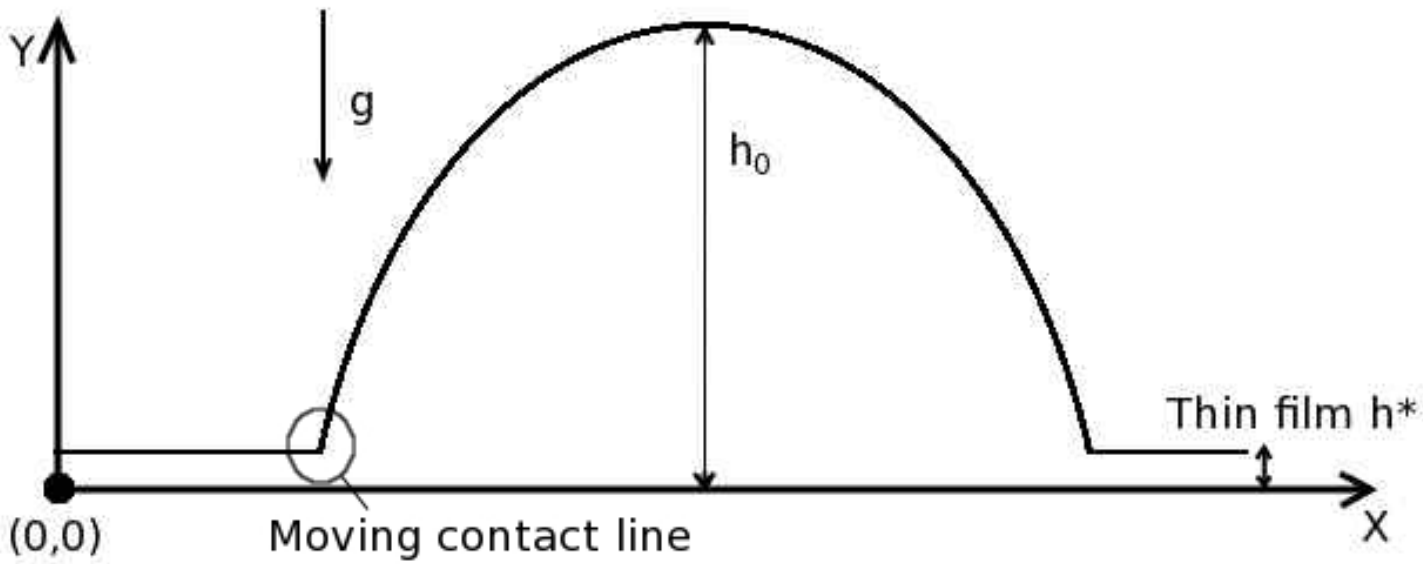


Droplet spreading model

$$\begin{aligned} \frac{\partial h}{\partial t} &= \frac{\partial}{\partial x}\left[\frac{h^3}{3}\left(\frac{\partial p}{\partial x} - \frac{B_o}{\epsilon} sin\alpha\right)\right] + \frac{\partial}{\partial y}\left[\frac{h^3}{3}\left(\frac{\partial p}{\partial y}\right)\right] \\ p &= -\triangle(h) - \Pi(h) + B_o h \cos\alpha \end{aligned}$$

with Neumann boundary conditions:

$$\partial_n h = 0 \quad \partial_n p = 0 \quad \text{on} \quad \partial\Omega$$

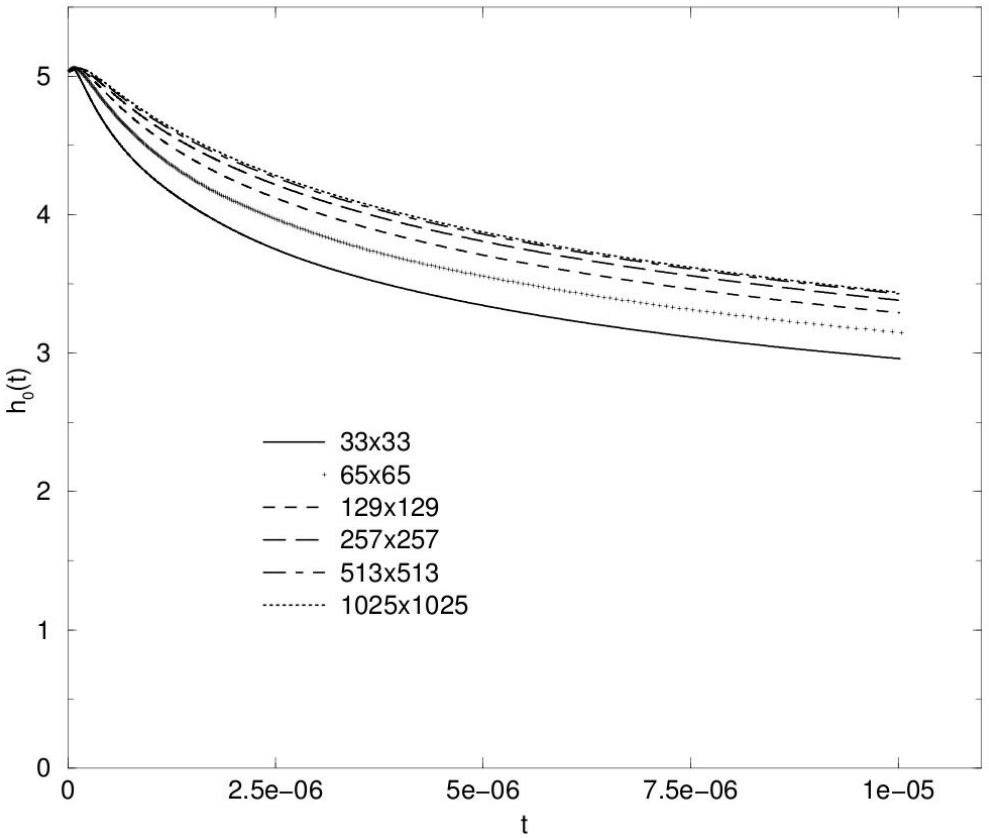


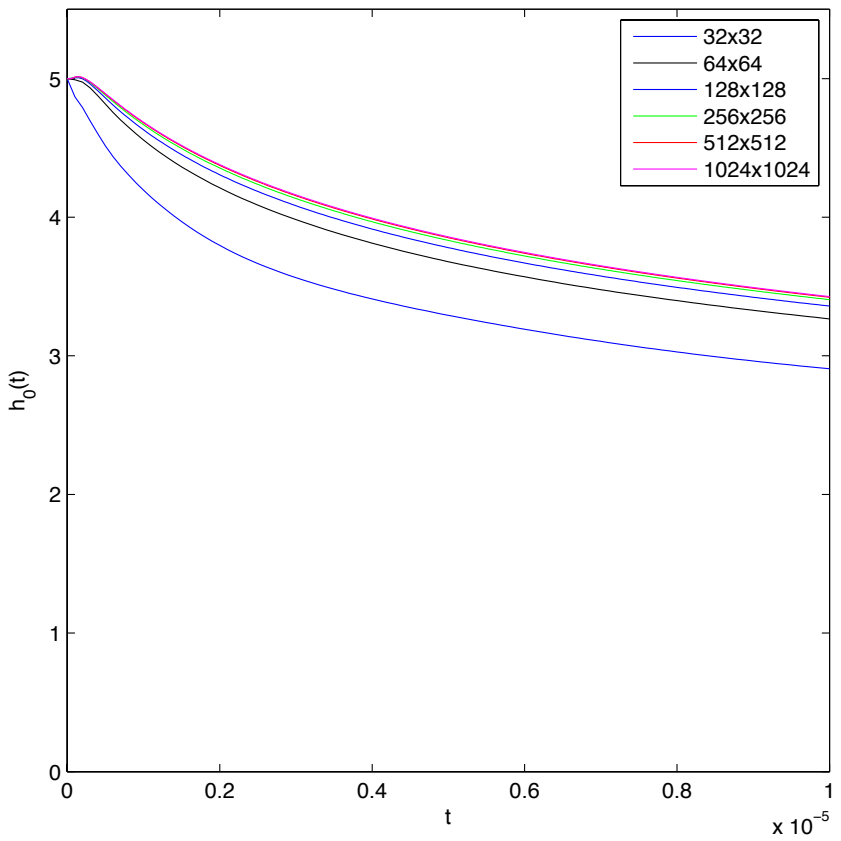
Gaskell et al. *Int. J. Numer. Meth. Fluids*, 45:1161-1186, 2004

Our solver

- Cell-centred 2^{nd} order finite difference method
- PARAMESH library for mesh generation and AMR
- Fully implicit BDF2 method with adaptive time-stepping
- MLAT variation of FAS multigrid at each time-step
- Newton-block 2×2 Red-Black (weighted) Gauss-Seidel smoother
- Full weighting restriction and bilinear interpolation
- Parallelism achieved using ARC2

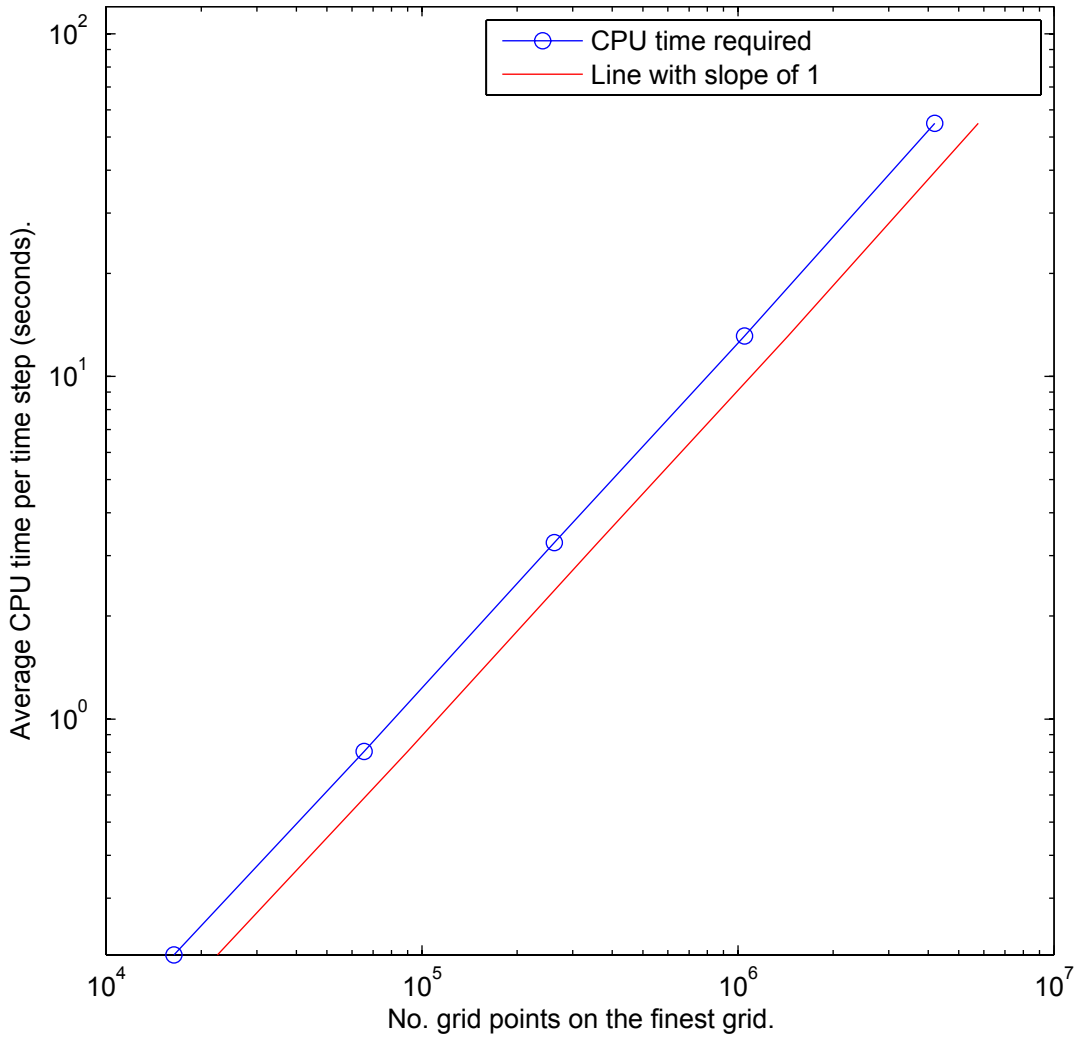
Validation





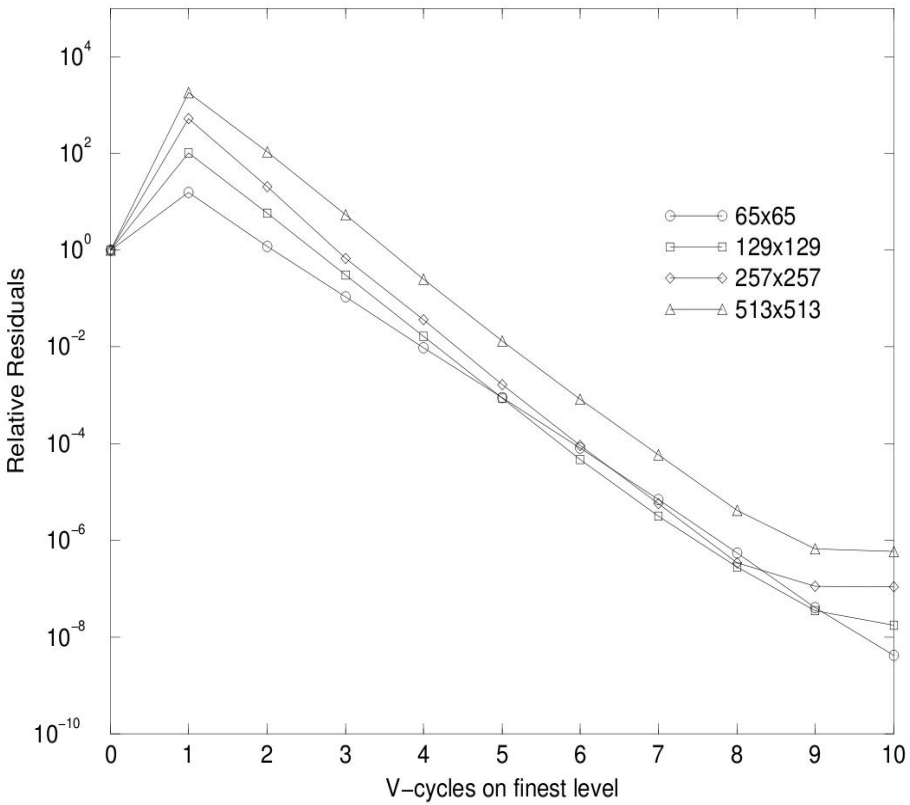
Results from Gaskell et al. on the left and our results on the right.

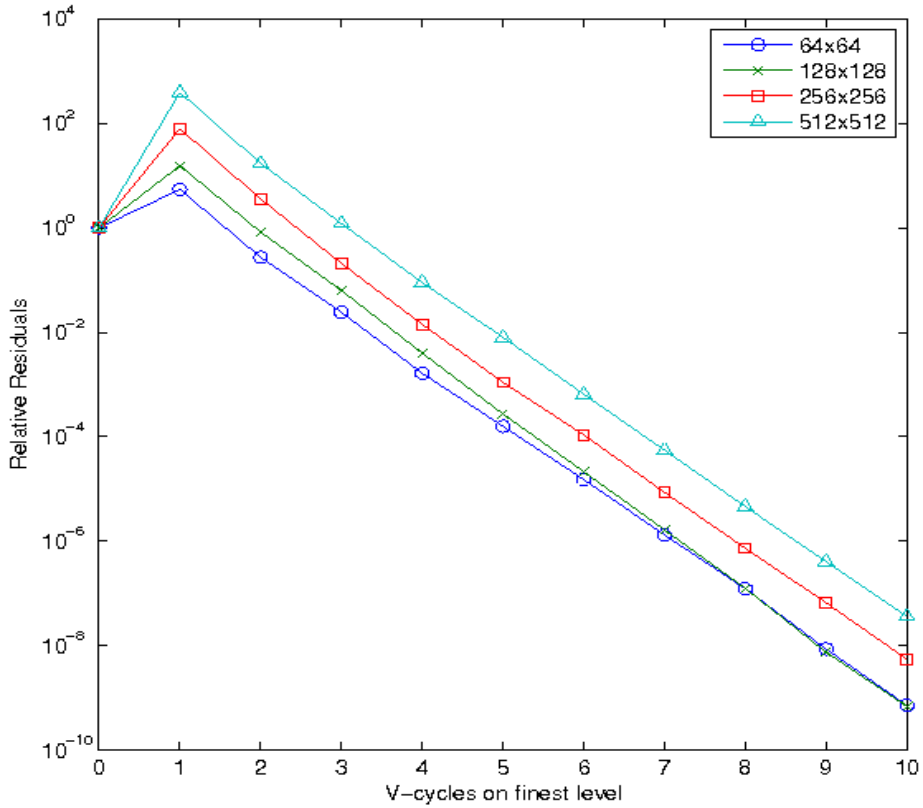
Multigrid linear complexity



A log-log plot demonstrating the linear complexity of multigrid.

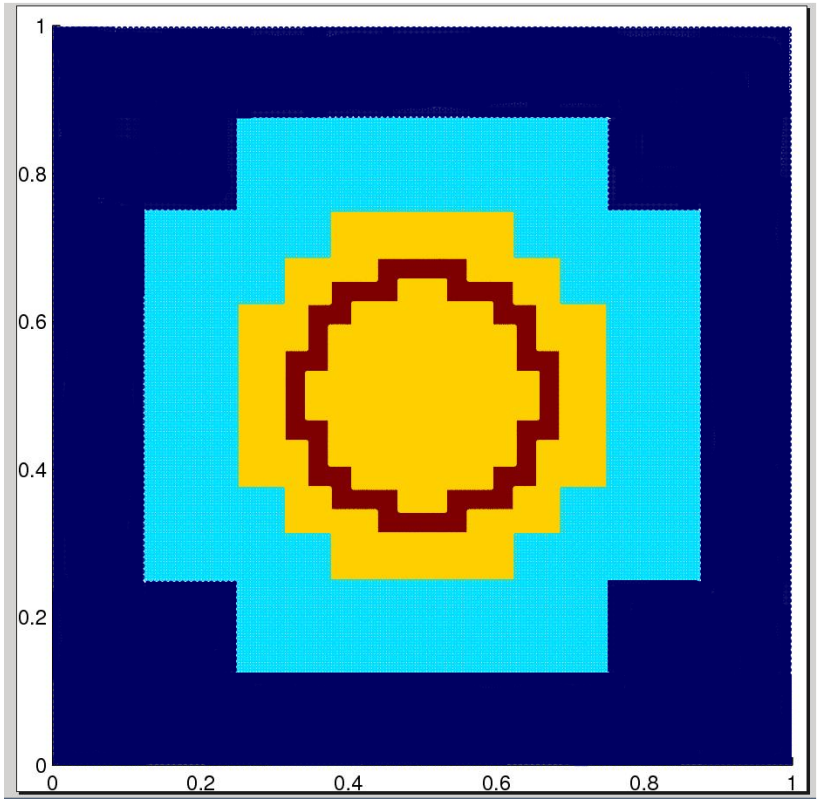
Multigrid performance

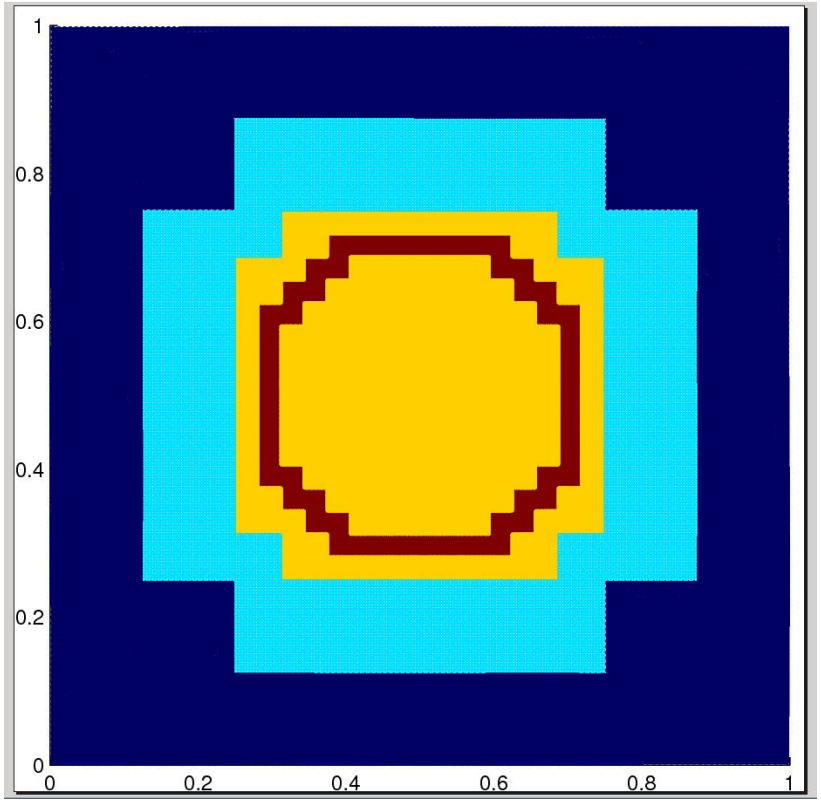




Results from Gaskell et al. on the left and our results on the right.

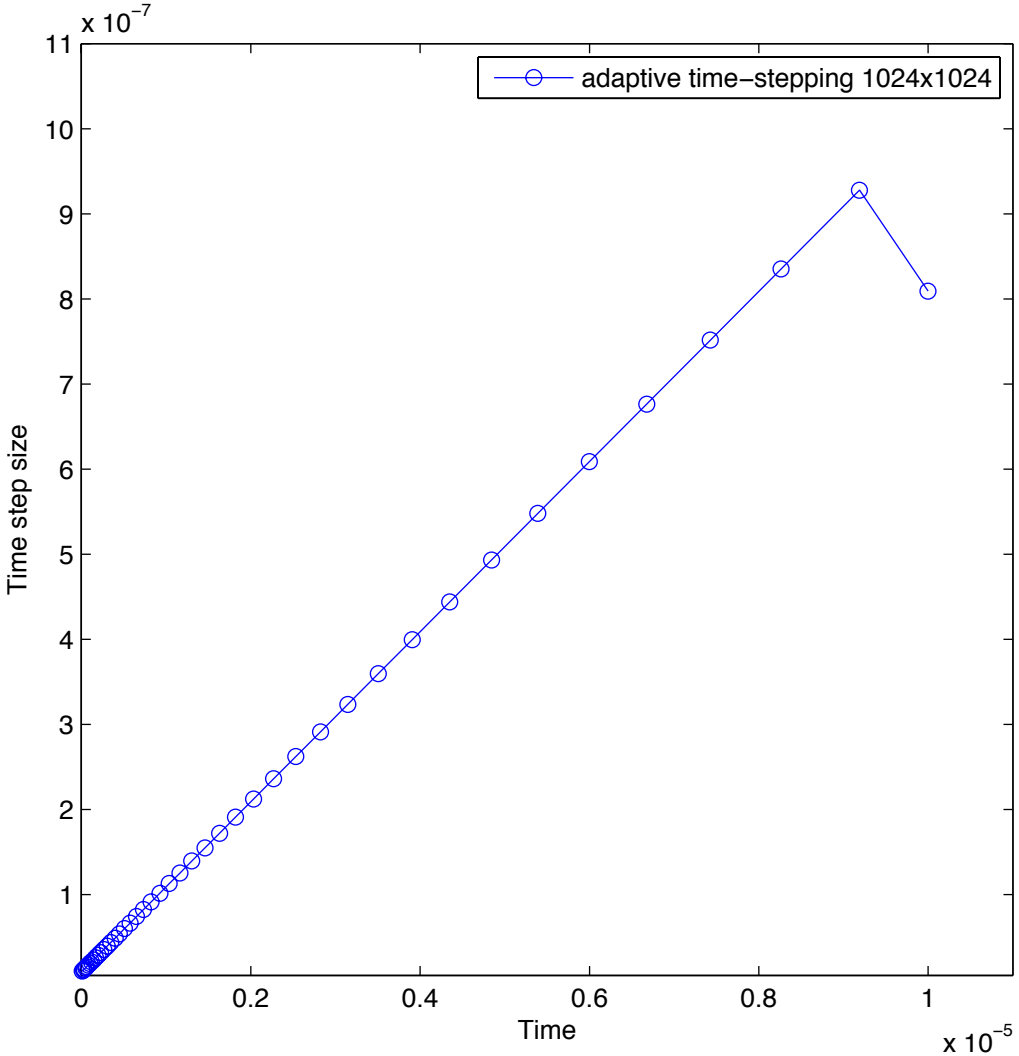
AMR





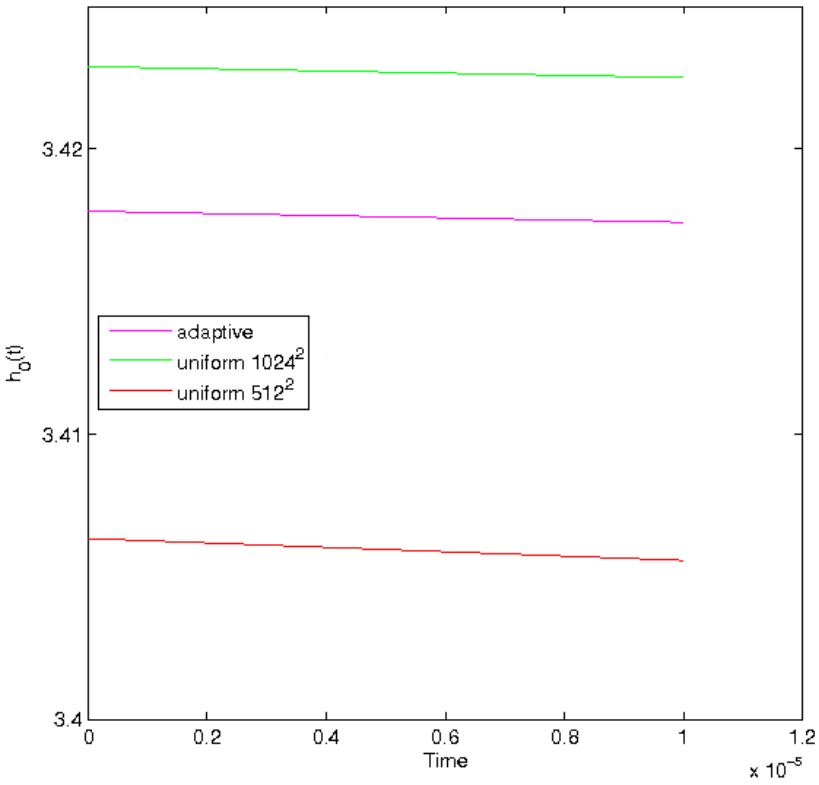
AMR with initial condition on the left and final solution on the right.

Adaptive time-stepping



Evolution of δt during $T = [0, 1 \times 10^{-5}]$.

Adaptive multigrid solver



Cases	No. leaf nodes
Uniform 1024^2	1,048,576
AMR	168,480

Cases	No. time steps	CPU time (seconds)
Fixed δt	1000	16721.3
ATS	45	574.4

Multigrid in parallel

No. cores	1	2	4	8	16	32	64
CPU time (seconds)	3282.6	1687.1	843.5	774.1	490.6	348.6	368.3

Table: A grid hierarchy $16 \times 16 - 1024 \times 1024$, and mesh block size is 8×8.

No. cores	1	2	4	8	16	32	64
CPU time (seconds)	3264.1	1625.1	840.1	687.3	439.5	351.2	301.7

Table: Another grid hierarchy of $32 \times 32 - 1024 \times 1024$, and mesh block size of 8×8.

Fully-developed flow

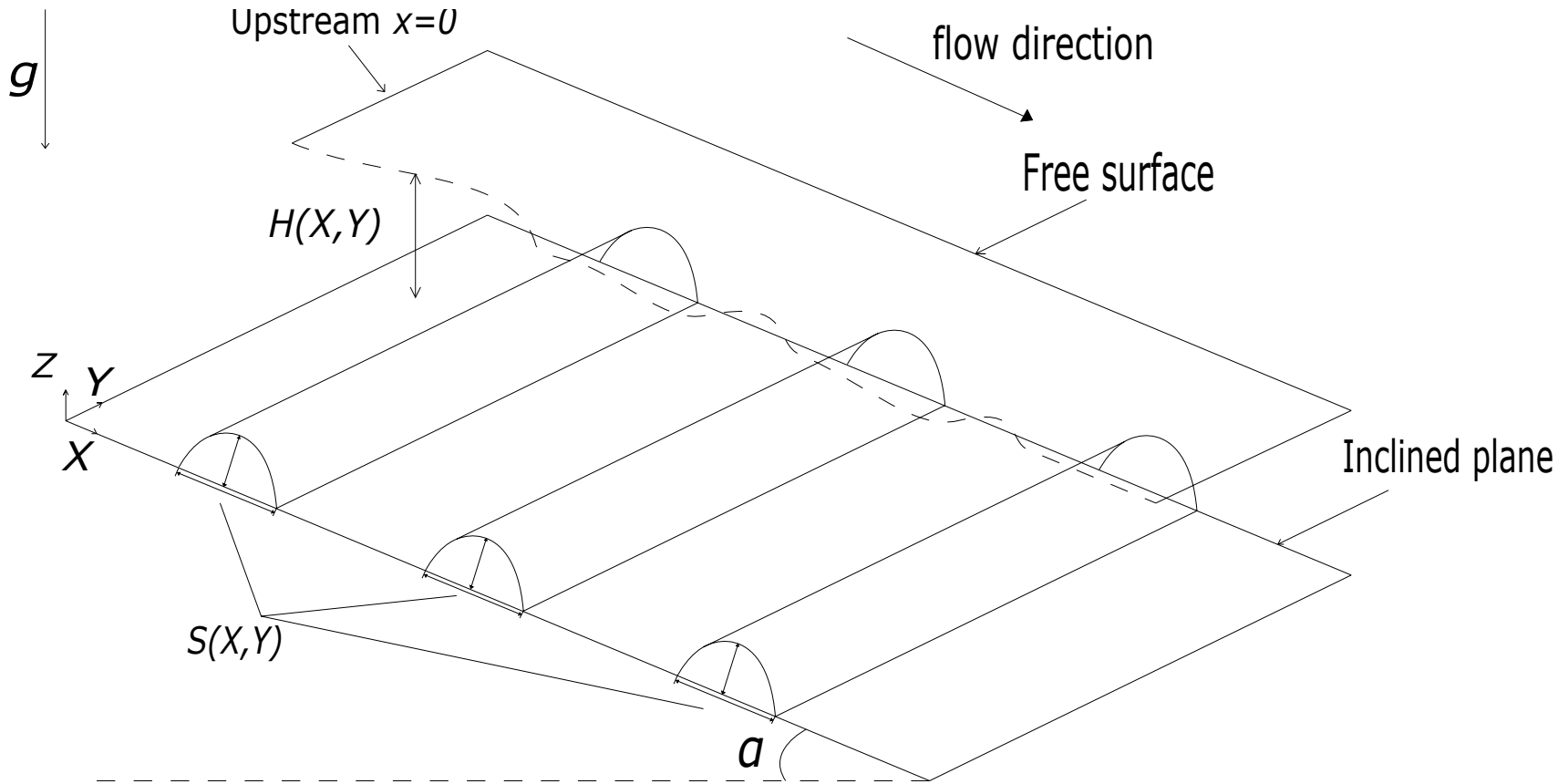
$$\begin{aligned} \frac{\partial h}{\partial t} &= \frac{\partial}{\partial x}\left[\frac{h^3}{3}\left(\frac{\partial p}{\partial x} - 2\right)\right] + \frac{\partial}{\partial y}\left[\frac{h^3}{3}\left(\frac{\partial p}{\partial y}\right)\right] \\ p &= -6\triangle(h+s) + 2\sqrt[3]{6}N(h+s) \end{aligned}$$

with mixed boundary conditions:

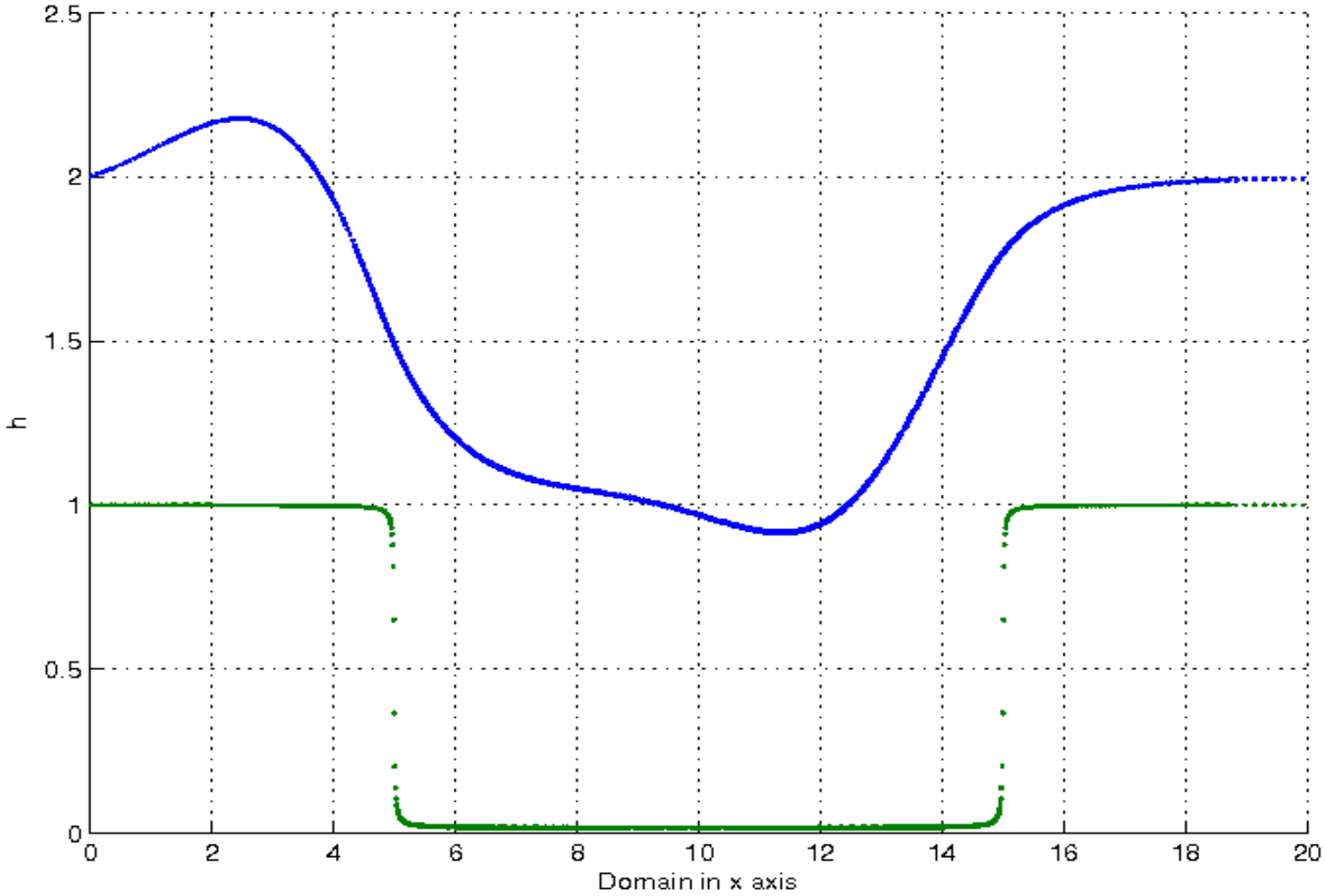
$$h(x=0,y) = g, \quad \frac{\partial p}{\partial x}|_{x=0} = 0, \quad \frac{\partial h}{\partial x}|_{x=1} = \frac{\partial p}{\partial x}|_{x=1} = 0,$$
$$\frac{\partial p}{\partial y}|_{y=0} = \frac{\partial p}{\partial y}|_{y=1} = \frac{\partial h}{\partial y}|_{y=0} = \frac{\partial h}{\partial y}|_{y=1} = 0.$$

Gaskell et al. *J. Fluids Mech*, 509:253-280, 2004

Sketch of the fully-developed flow



Our results with a trench topography



Cahn-Hilliard-Hele-Shaw system of equations

$$\begin{aligned}
\frac{\partial \phi}{\partial t} &= \triangle \mu - \nabla \cdot (\phi \boldsymbol{u}), \\
\mu &= \phi^3 - \phi - \epsilon^2 \triangle \phi, \\
\boldsymbol{u} &= -\nabla p - \gamma \phi \nabla \mu, \\
\nabla \cdot \boldsymbol{u} &= 0,
\end{aligned}$$

with Neumann boundary conditions:

$$\partial_n \phi = \partial_n \mu = \partial_n p = 0 \quad \text{on} \quad \partial\Omega,$$

Wise *J. Sci. Comput.*, 44:38-68, 2010

Cahn-Hilliard-Hele-Shaw system of equations

$$\begin{aligned} \frac{\partial \phi}{\partial t} &= \nabla \cdot (M(\phi)\nabla \mu) - \nabla \cdot (\phi \nabla p), \\ \mu &= \phi^3 - \phi - \epsilon^2 \triangle \phi, \\ -\triangle p &= \gamma \nabla \cdot (\phi \nabla \mu), \end{aligned}$$

with Neumann boundary conditions:

$$\partial_n \phi = \partial_n \mu = \partial_n p = 0 \quad \text{on} \quad \partial\Omega,$$

Wise *J. Sci. Comput.*, 44:38-68, 2010

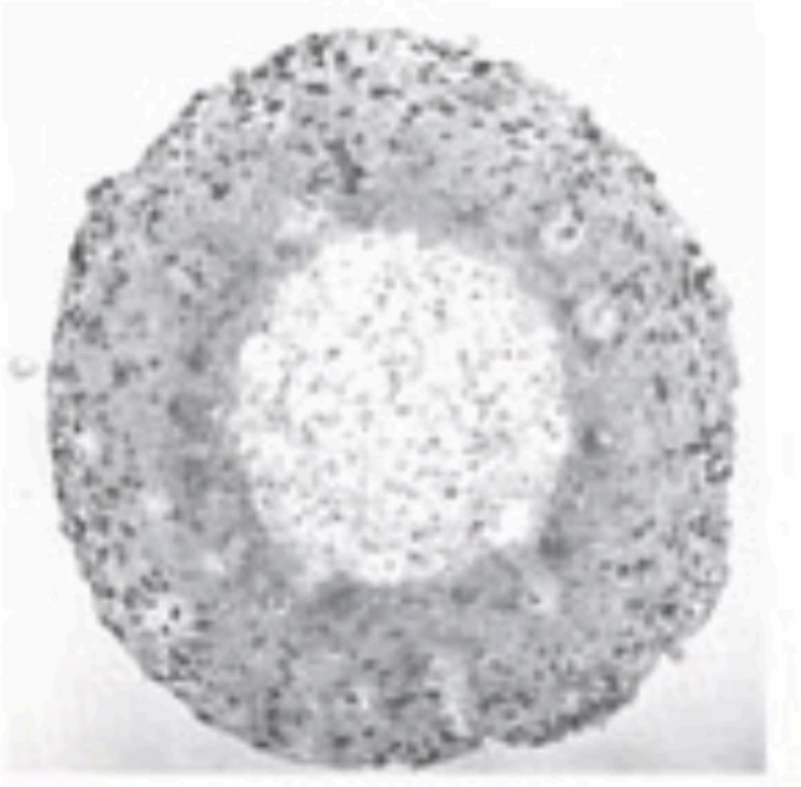
2^{nd} order convergence rate

For variable ϕ					
Levels	Time steps	Infinity norm	Ratio	Two norm	Ratio
3	40	-	-	-	-
4	80	1.074×10^{-3}	-	3.885×10^{-4}	-
5	160	2.718×10^{-4}	3.95	9.781×10^{-5}	3.97
6	320	6.905×10^{-5}	3.93	2.468×10^{-5}	3.96

Table: 2^{nd} order convergence rate seen from CHHS system of equations.

Tumour modelling - avascular tumour growth

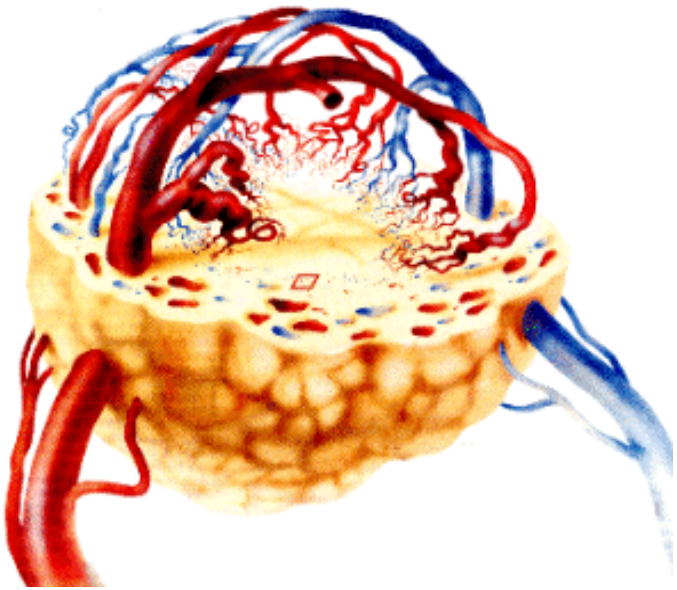
- Starts with a small cluster of cells
- Nutrient supply through diffusion
- Internal adhesion force
- Three layers of cells:
  - Proliferative cells
  - Dormant cells
  - Dead cells (necrosis)
- Volume loss in necrotic core



source: *www.bioinfo.de*

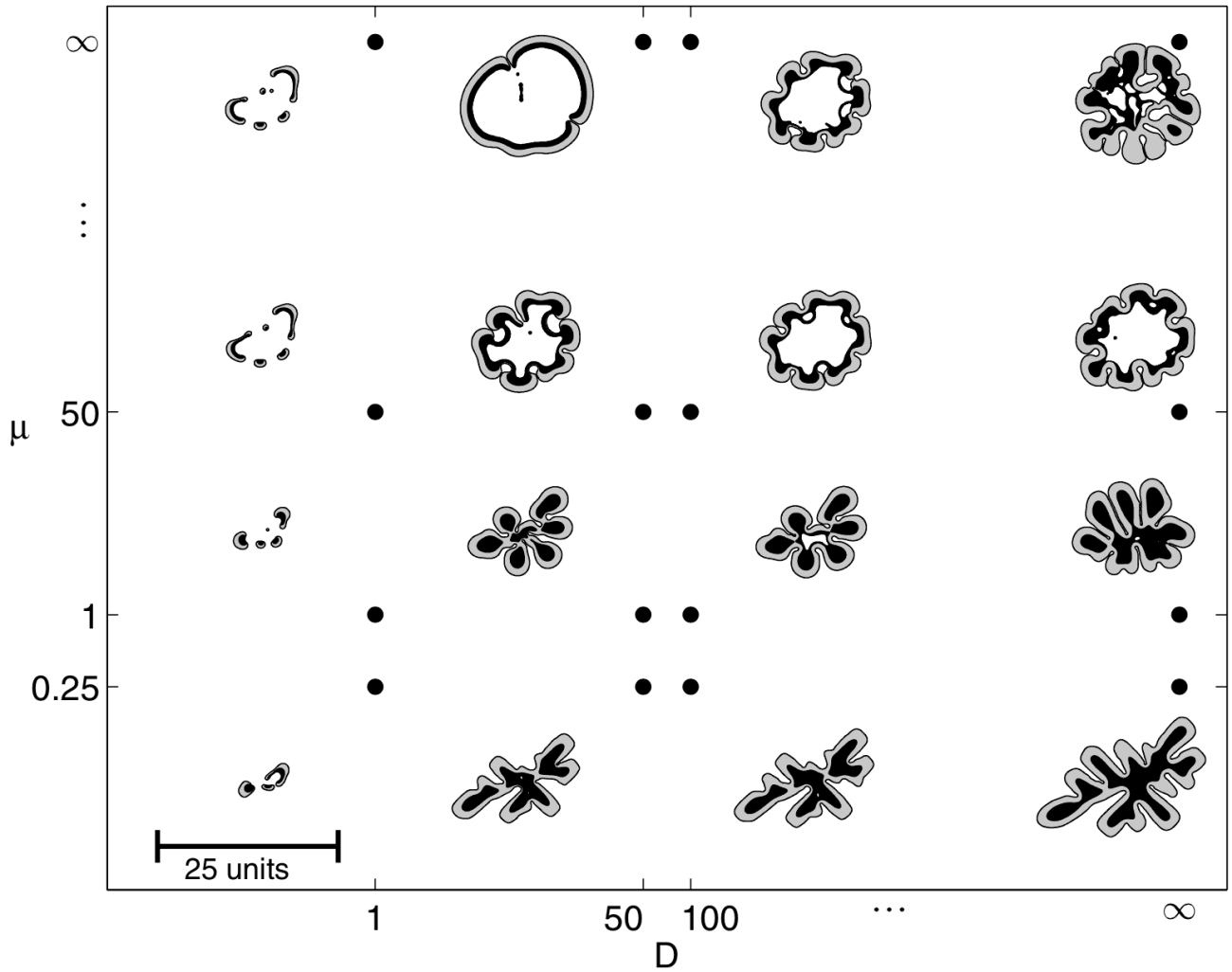
Tumour modelling - vascular tumour growth

- TAF chemical factor
- Inducing blood vessel (angiogenesis)
- Exponential growth rate
- Develop secondaries through metastasis



source: *www.maths.dundee.ac.uk*

Tumour modelling - micro-environments



J. S. Lowengrub, H. B. Frieboes, Y-L. Chuang, F. Jin, X. Li P. Macklin, S. M. Wise,

Nonlinearity 23:R1-R91, 2010

Tumour model from Wise et al.

$$
\begin{aligned}
\partial_t \phi_T &= M\nabla \cdot (\phi_T \nabla \mu) + S_T(\phi_T, \phi_D, n) - \nabla \cdot (\mathbf{u_S} \phi_T) \\
\mu &= f'(\phi_T) - \epsilon^2 \Delta \phi_T \\
\partial_t \phi_D &= M\nabla \cdot (\phi_D \nabla \mu) + S_D(\phi_T, \phi_D, n) - \nabla \cdot (\mathbf{u_S} \phi_D) \\
\mathbf{u_S} &= -(\nabla p - \frac{\gamma}{\epsilon} \mu \nabla \phi_T) \\
\nabla \cdot \mathbf{u_S} &= S_T(\phi_T, \phi_D, n) \\
0 &= \Delta n + T_C(\phi_T, n) - n(\phi_T - \phi_D)
\end{aligned}
$$

with mixed boundary conditions:

$$\mu = p = 0 \;\; n = 1 \;\; \partial_n \phi_T = \partial_n \phi_D = 0 \;\; \text{on} \;\; \partial\Omega,$$

S. M. Wise, J. S. Lowengrub, V. Cristini,

Math. Comput. Modelling, 53: 1-20, 2011.

Tumour model from Wise et al.

$$
\begin{aligned}
\partial_t \phi_T &= M\nabla\cdot(\phi_T\nabla\mu) + S_T(\phi_T,\phi_D,n) - \nabla\cdot(\mathbf{u_S}\phi_T) \\
\mu &= f'(\phi_T) - \epsilon^2\Delta\phi_T \\
\partial_t \phi_D &= M\nabla\cdot(\phi_D\nabla\mu) + S_D(\phi_T,\phi_D,n) - \nabla\cdot(\mathbf{u_S}\phi_D) \\
[\mathbf{u_S} &= -(\nabla p - \frac{\gamma}{\epsilon}\mu\nabla\phi_T)] \\
-\Delta p &= S_T(\phi_T,\phi_D,n) - \nabla\cdot(\frac{\gamma}{\epsilon}\mu\nabla\phi_T) \\
0 &= \Delta n + T_C(\phi_T,n) - n(\phi_T-\phi_D)
\end{aligned}
$$

with mixed boundary conditions:

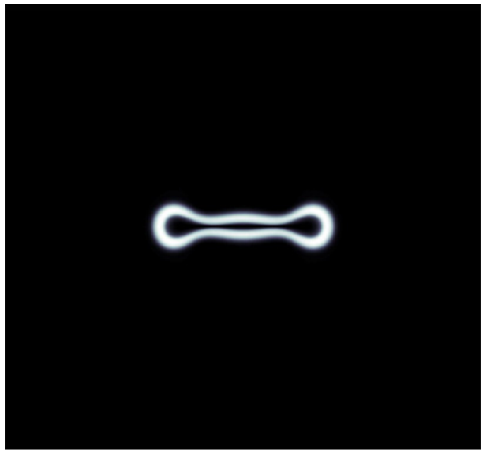
$$\mu = p = 0 \;\; n = 1 \;\; \partial_n\phi_T = \partial_n\phi_D = 0 \;\text{ on }\; \partial\Omega,$$

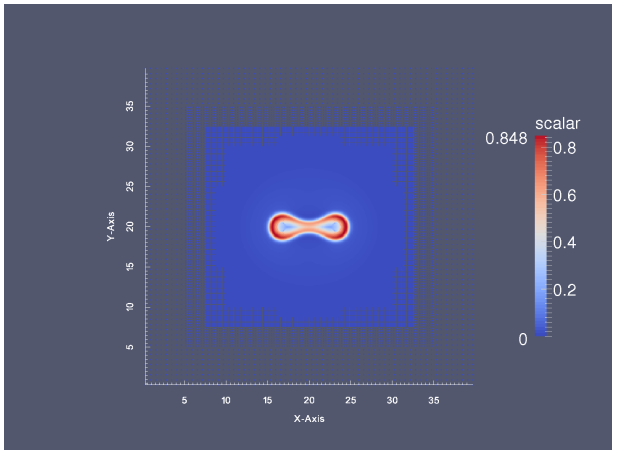
S. M. Wise, J. S. Lowengrub, V. Cristini,

Math. Comput. Modelling, 53: 1-20, 2011.

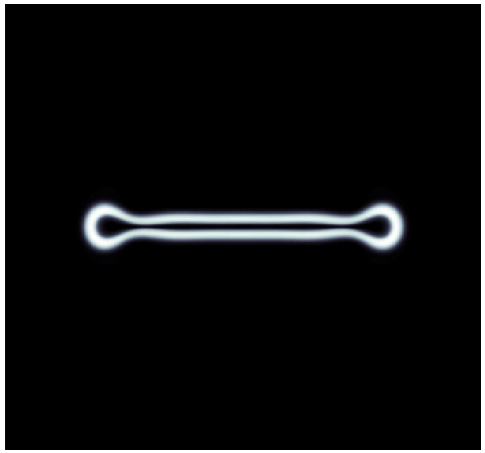
Validation

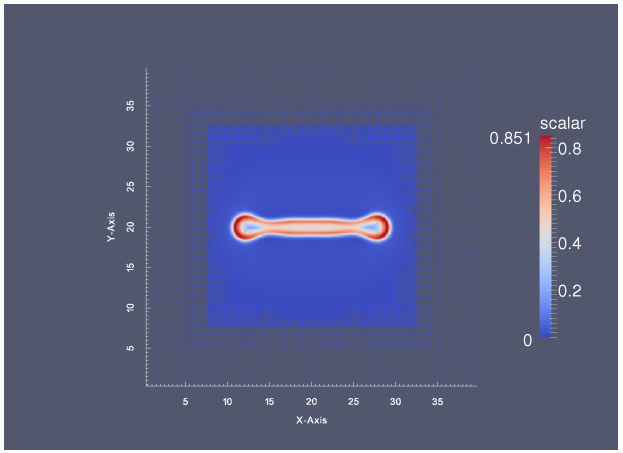
t=100





t=200





Validation between results of Wise et al. and ours.

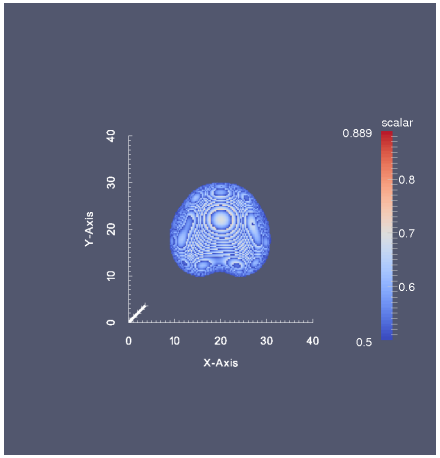
2^{nd} order convergence rate

For variable ϕ_T					
Levels	Time steps	Infinity norm	Ratio	Two norm	Ratio
$5(128^2)$	1250	-	-	-	-
$6(256^2)$	2500	9.118×10^{-2}	-	7.836×10^{-3}	-
$7(512^2)$	5000	1.322×10^{-2}	6.90	1.131×10^{-3}	6.93
$8(1024^2)$	10000	2.579×10^{-3}	5.13	2.367×10^{-4}	4.78
$9(2048^2)$	20000	6.415×10^{-4}	4.02	5.833×10^{-5}	4.06

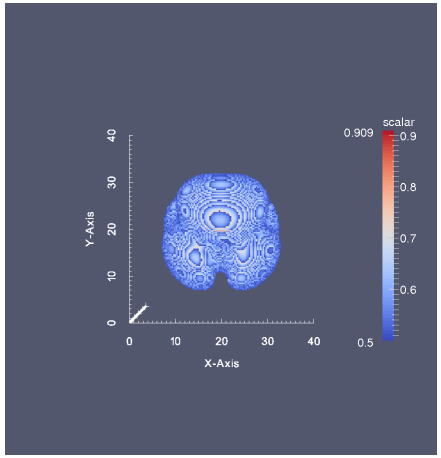
2^{nd} order convergence rate seen from the model of tumour growth.

3-D results

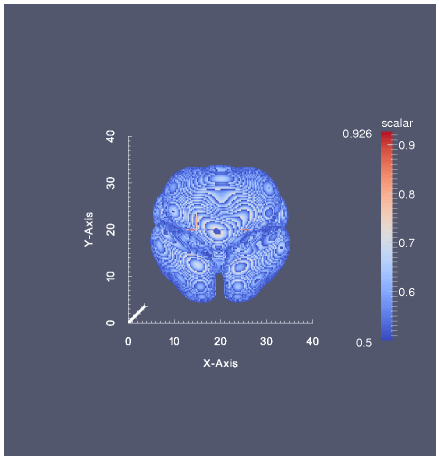
t=50



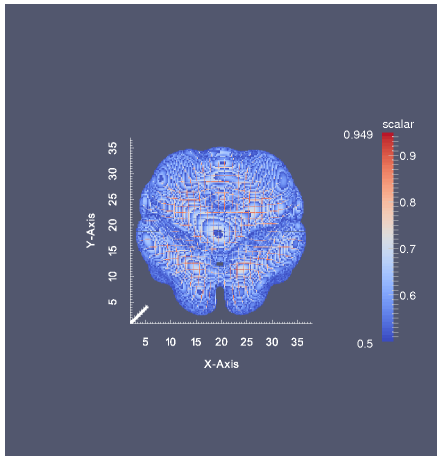
t=100



t=150

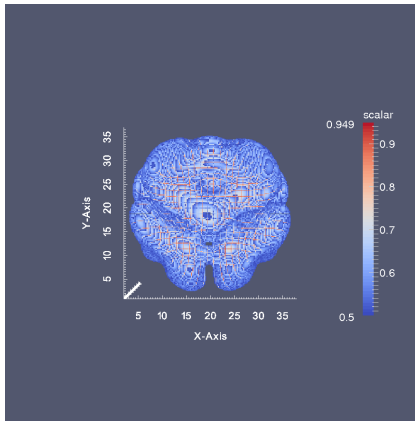


t=200

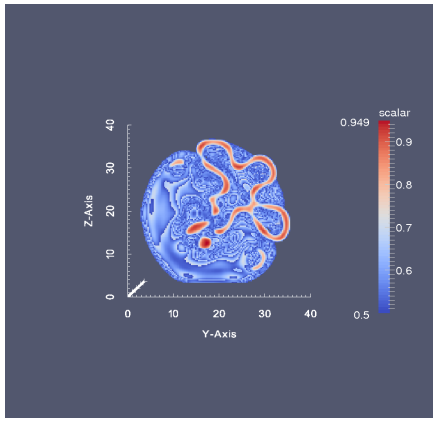


3-D results

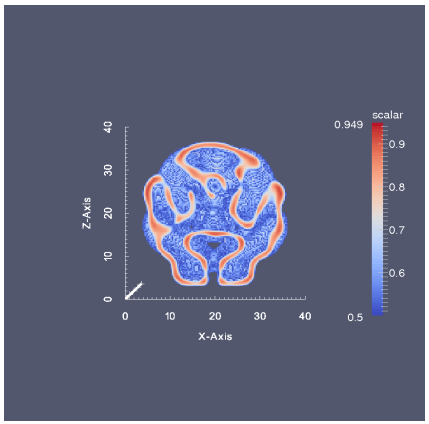
t=200



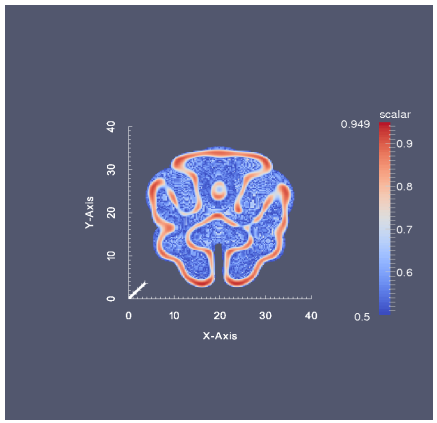
Cutting through x plane



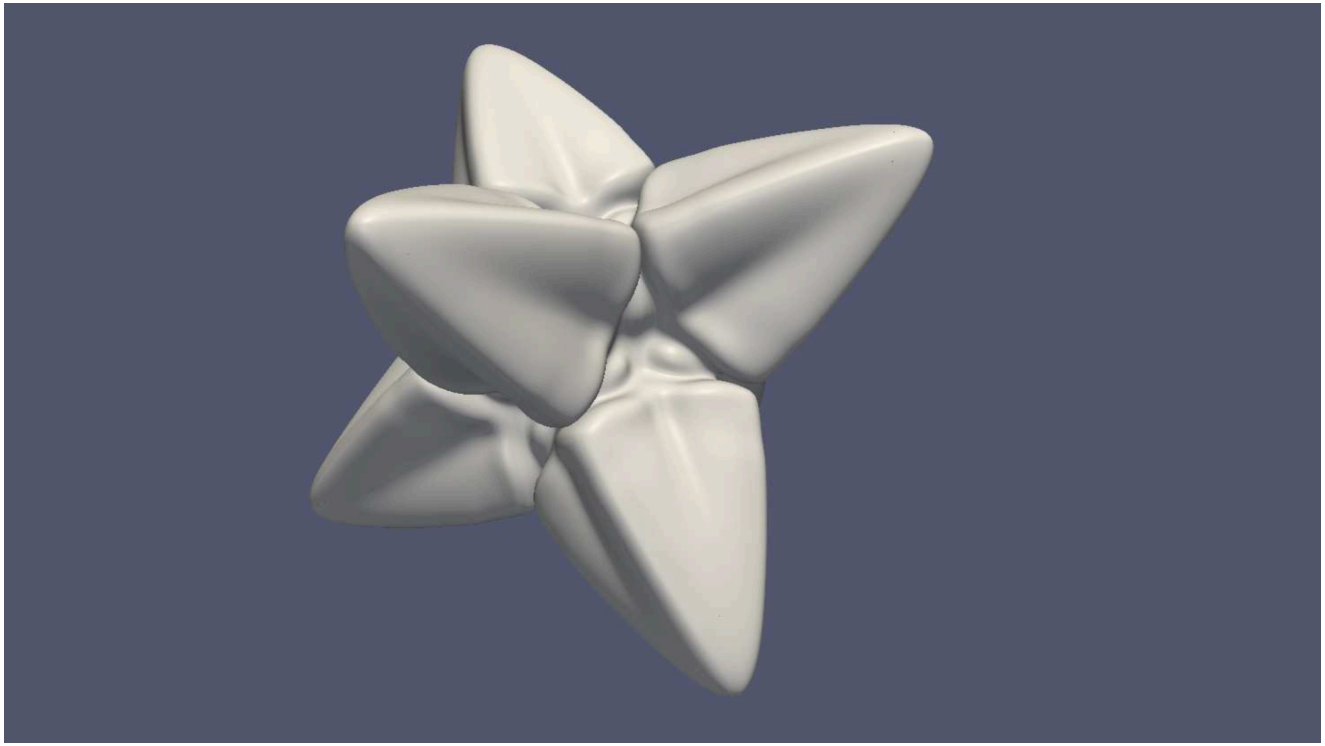
Cutting through y plane



Cutting through z plane



The End



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